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# Raman spectroscopy of graphene trilayers with different stacking orders

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Graphene multilayers have received significant theoretical and experimental attention in recent years. Raman scattering has become a particularly useful way to study these materials, allowing one to determine the number of monolayers, strains within them, their level of doping, and the concentration of defects. However, one thing that Raman spectroscopy has not yet been used to study is the stacking configuration of graphene in multilayers. In this paper, we investigate the shape of the 2D Raman mode in ABA and ABC stacked graphene trilayers. It was found that the 2D mode is asymmetric in ABC regions and symmetric in ABA regions. Additionally, we use Raman scanning to find a quantifier that allows us to map ABA and ABC stacking domains. Using statistical analysis, we find that the most effective quantifiers are the line width of the 2D mode and the spectrally integrated residual between the recorded Raman spectrum and the ABC mode. While other parameters that we considered vary between the different stacking regions also, the changes in them are insignificant compared to the measurement uncertainty.

Graphene is a one atom-thick sheet of  $sp^2$ -hybridized carbon atoms, arranged in a hexagonal lattice. The material has been of great theoretical interest since the mid 1900s [1], mainly due to its interesting charge transport properties. Theoretical studies have shown that the dispersion relationship for graphene is conical at low energies, implying that electrons in the material's lattice have a zero effective mass. In particular, graphene's conduction-band electrons behave like relativistic particles, whose behavior is governed by the Dirac equation [2]. Interestingly, it was theorized by Landau that a 2-dimensional crystal like graphene would be thermodynamically unstable [3]. Therefore, it was thought that the production of the material would be impossible. However, the successful production of graphene was accomplished in 2004, by Andre Geim *et al.* [4]. It has since been theorized that corrugations and ripples on the atomic scale might be responsible for the thermodynamic stabilization of graphene sheets [5].

Since the initial production of graphene in 2004, many applications have been realized for both monolayers and bilayers. The driving force behind monolayer applications is graphene's high intrinsic carrier mobility at room temperature [6]. This has made the material favorable in many potential technological devices including nano-ribbon field effect transistors (GNRFETs) [7] and radio-frequency (RF) transistors [1]. The number of potential applications involving bilayer graphene is also quite high. This is a result of the materials interesting band-structure, which arises from electronic interactions between graphene layers. In particular, it was found that an electric field, applied perpendicular to the bilayer, can open a band gap [8,9]. This makes bilayers useful in gated devices, such as FETs, which are ubiquitous in modern microelectronics.

While graphene monolayers and bilayers have been studied quite thoroughly, trilayers have not received much experimental attention. The main complexity in studying them arises from the fact that there are two stable stacking orders: ABA and ABC. Although the difference between these stacking configurations is quite subtle, theoretical studies predict that they have completely different band structures, at low energies. These studies show that ABA-stacked trilayers are semi-metals, with finite band overlap, while ABC-stacked trilayers are zero-gap semi conductors [10]. For consistent results in future studies, it is important for one to be able to distinguish between these stacking orders. Therefore, to provide this groundwork, we must find a method for the effective characterization of trilayers.

To date, several characterization techniques have been prominent in monolayer and multilayer studies. Atomic force microscopy (AFM) has been used to study the number of layers in few-layer samples, along with their morphology. Although this technique is useful, it has been cited as unreliable [11]. Another method, which also allows us to determine the number of layers, is transmission electron microscopy (TEM). While TEM is more reliable than AFM, it requires the sample to be suspended, which is often impractical. The presence of optical transitions in the infrared (IR) range for multilayers offers us a useful new way to study them. IR spectroscopy allows us to probe the electronic band structure, which gives us access to a wealth of information that cannot be determined from either AFM or TEM data. Recent theoretical studies have shown that high-energy IR (NIR) measurements can be used to determine the number of layers in a multilayer, and lower-energy IR (MIR) measurements can be used to determine the stacking

order [12]. While IR is more reliable and practical than TEM and AFM, as well as more informative, it is not available in most research laboratories. Raman scattering, on the other hand, has not been met with the difficulties described above. The method is reliable, practical, and is available in most research laboratories. Therefore, it is most beneficial for us to study the Raman spectrum of graphene trilayers, in attempt to find ways to characterize as many physical features as possible.

To date, the Raman spectrum of graphene, and multilayers, has been used to characterize many physical features. The intensity of the D mode has allowed one to determine the quality of a sample [13]. The shape of the 2D overtone has been used to determine the number of layers in a multilayer [13]. The width of the G mode has allowed us to study the level of doping of a sample [14]. And finally, the shifts of the 2D and G modes, along with the width of the G mode, have allowed one to study the strain on a sample [15]. Although this information tells us a lot, there is still more to be inferred. To date, there is no clear consensus on the shape of the 2D mode in trilayer graphene. This mode is shown to have asymmetric features in some studies [16-18], and symmetric features in others [19-21]. In this study, we aim to resolve this inconsistency by considering the stacking order of trilayer graphene. Additionally, we look for a quantifier that allows us to map stacking domains from Raman scanning measurements.

## II. Experimental and Analytical Methods

Graphene multilayer samples were produced by the method of mechanical exfoliation of kish graphite [23]. Our substrate was Si coated with 300nm SiO<sub>2</sub>. Samples of reasonable shape and size were found with an optical microscope.

Raman spectroscopy was performed using a 532nm laser as the excitation source, with an 1800 slit/cm grating, and a resulting spectral resolution of  $\sim 0.6\text{cm}^{-1}$ . The integration time per spectrum was set at 8 minutes. Infrared spectroscopy was performed on a micro-FTIR apparatus with a Globar source and a HgCdTe detector in Brookhaven National Laboratory. 2D Raman mapping was performed using 514.5nm linearly polarized light from an Argon laser. Raman spatial maps were taken with a spot size of roughly 500nm, a step size of 500nm, and a resolution of  $8\text{cm}^{-1}$ . The integration time was fixed at 5 seconds.

Within the Results and Discussion, we refer to several parameters. The central frequency ( $\langle\omega\rangle$ ) is given by the statistical relationship in Eq. 1., where  $\omega$  is the frequency and  $I(\omega)$  is the Raman intensity at that frequency.

$$\langle\omega\rangle = \frac{\int \omega \cdot I(\omega) \cdot d\omega}{\int I(\omega) \cdot d\omega} \quad (1)$$

An asymmetry parameter was calculated by integrating each half of the 2D mode and then taking their ratio. The mathematical formulation of this procedure is given in Eq. (2). Here  $\omega_L$  and  $\omega_R$  are the frequencies at which the mode reaches 15% of its maximum intensity.  $I_L$  and  $I_R$  are the values of the left and right integrals.

$$\frac{I_R}{I_L} = \frac{\int_{(\omega_L + \omega_R)/2}^{\omega_R} I(\omega) \cdot d\omega}{\int_{\omega_L}^{(\omega_L + \omega_R)/2} I(\omega) \cdot d\omega}, \omega_R > \omega_L \quad (2)$$

A so-called residual parameter ( $\eta$ ) was also calculated. This was done by subtracting the spectrum of the ABC stacked 2D mode ( $I_{ABC}(\omega)$ ) from the measured spectra ( $I(\omega)$ ), and then integrating the resulting spectrum over  $\omega$  (see Eq. 3). The ABC stacked 2D mode will be discussed within the Results and Discussion section.

$$\eta = \int |I_{ABC}(\omega) - I(\omega)| d\omega \quad (3)$$

The line width ( $\Gamma$ ) was calculated as the width of the 2D mode at  $3/4$  of maximum intensity. Statistical analysis was performed in MATLAB using a mixture of original code and built in functions (see **Appendix A5** for complete code).

## III. Results and Discussion

In a recent study, it was found that the transmission plateau in the NIR spectrum of multilayers is quantized with respect to layer number [12]. This results from the hyperbolic bands that make up multilayer's band structures. In NIR energy ranges, the bands run parallel to one another, along their respective asymptotes.

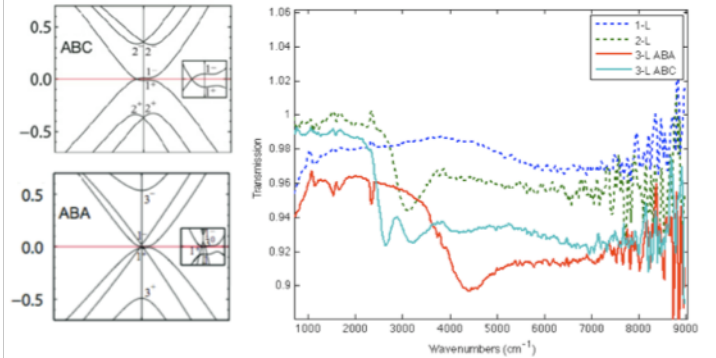


FIG. 1. (a)-(b) Band structures of ABC and ABA stacked trilayers [10]. (c) The IR spectra of monolayers, bilayers, and trilayers with ABA and ABC stacking geometry. The NIR tails of the teal and red curves tell us that both curves are representative of trilayers. The MIR transmission peaks tell us the stacking type.

Qualitatively, this situation is analogous to having multiple monolayers with linear bands. Furthermore, in a trilayer such an arrangement will result in roughly triple the absorption of a monolayer. After finding trilayers in this way, we looked to the lower energy transmission spectrum. In accord with the literature, we found only two distinctly different MIR transmission patterns, with converging tails in the NIR range. Theoretical studies have shown that ABA and ABC stacked trilayers are the most energetically favorable [23]. To determine which spectrum corresponds to which stacking geometry, we studied the trilayer band structure. It turns out that two strong MIR absorption features are possible with ABC geometry and only one with ABA geometry. Indeed one class of spectra had one transmission peak while the other had two transmission peaks, making it feasible to make the distinction. These results are summarized in Fig. 1.

A sample was found with both stacking orders, and the locations of these domains were determined by performing multiple IR measurements. Raman measurements were then taken within each domain, so as to determine the shapes of the 2D modes in ABA and ABC stacked regions (see Fig. 2, where we have the averaged several spectra from ABA and ABC regions). Although both curves in the figure display some oscillatory noise, they are clearly distinct. The ABC domain produces an asymmetric 2D mode, with a pronounced peak, while the ABA domain produces a more symmetric mode with a broad peak. Additionally it appears that the ABC mode is wider than the ABA mode by several wavenumbers. As already mentioned, curves similar to those presented here have appeared in the literature. However, they have never been presented simultaneously, and there has not been any inquiry as to what physical features are responsible for the variation in their shapes. From the combination of our IR and Raman data, it becomes clear that these two shapes are the signatures of ABA and ABC stacking geometries. After clarifying this fact, it was our goal to quantify these

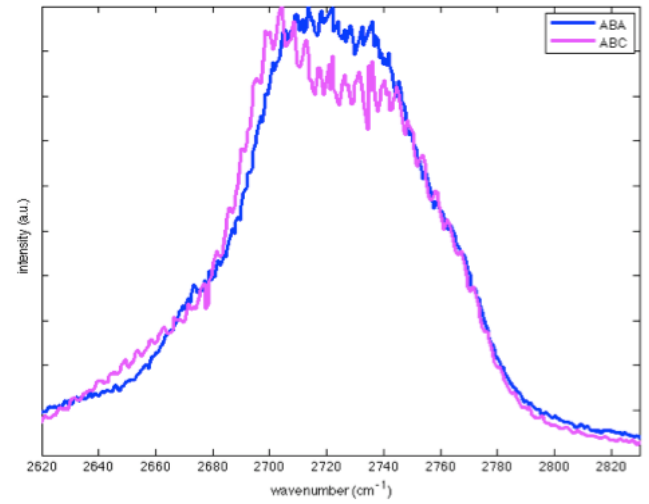


FIG. 2. Raman spectra of graphene trilayers with ABA and ABC stacking geometries. Stacking geometry was confirmed with IR measurements. The ABC produced mode is asymmetric and has a greater width than the ABA mode. The ABA produced mode is more symmetric with a smooth peak.

shape differences, and to map stacking domains.

To facilitate this study, we acquire Raman spectra while raster-scanning the sample along a 46 by 110 grid. Several quantities were calculated at each pixel and plotted in the form of colormaps (each pixel corresponds to a single spectrum). Each quantity attempts to capture the apparent difference between the 2D mode in ABA and ABC domains in a different way. First, we calculated the central frequency of the mode, by applying Eq. (1). (see Fig. 3(b)). The leftward asymmetry of the ABC mode should cause this to register a lower central frequency than a symmetric mode. Then, we calculated the asymmetry parameter, as given by Eq. (2). In symmetric modes, such as those that arise in ABA regions, this quantity should be close to 1. However, in asymmetric regions, such as those with ABC

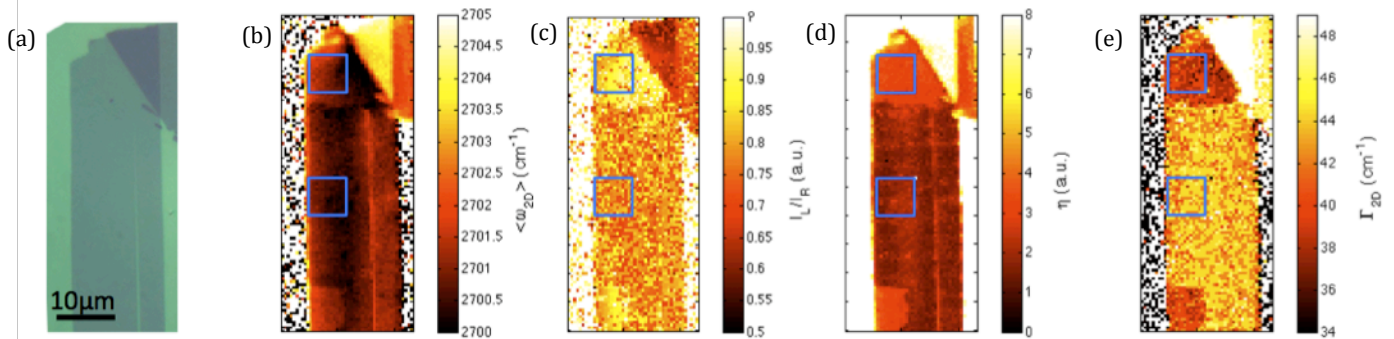


FIG. 3. (a) optical photograph of our trilayer sample. The scale bar represents 10μm. (b) The central frequency of the 2D mode. (c) The ratio of the integrated intensities of the left hand side of the mode to the right hand side (d) The residual at each point. (e) The line width of the mode at  $\frac{3}{4}$  maximum. In these figures, prominently in (c) and (d), we see a sharp boundary, which is representative of stacking. The physical explanation for the gradually varying features in (b) has not yet been devised. The Blue squares represent areas where data was sampled for statistical analysis. The stacking in these blue regions was also confirmed by IR spectroscopy.

stacking, this ratio should be noticeably smaller than one. These results are plotted in Fig. 3(c). Next, the residual parameter was calculated, as given by Eq. (3) (see Fig. 3(d)). Asymmetric modes will return a small value for this parameter while symmetric modes will return a large value. Finally, to account for the apparent broadening in the ABC mode, we calculated the line width (denoted  $\Gamma_{2D}$ , see Fig. 3(b)).

In the obtained maps, we immediately notice the presence of several domains (see Fig. 3(b)-(e)). Note that the vertical line on the right-hand side of the sample is a structural artifact and can be seen in the optical photograph in Fig. 3(a). In these maps we clearly see a homogeneous ABC region at the center of the trilayer that separates two smaller ABA domains at the top and bottom parts of the sample. Indeed these are the same regions where IR and Raman measurements were taken, and where we have confirmed the presence of different stacking domains. Therefore, it appears that the carefully chosen parameters are effective. However, we also notice that some parameters are better than others in this mapping. In particular, we see a lot of noise in Fig. 3(e), and gradually varying features, that are not representative of stacking, in Fig. 3(a).

For further quantitative analysis, we have carefully examined 12x12 regions within homogeneous ABA and ABC domains (these grids are indicated by the blue squares in Fig. 3(b)-(e)). Histograms representing the distributions of the studied parameters, for each stacking domain, are plotted in Fig. 4. Each distribution was assumed normal and was fit with a Gaussian. See **Table 1** in **Appendix A4** for the mathematical parameters that describe these Gaussians. The purpose of this step was to determine the amount of overlap between the distributions. Each Gaussian was integrated from their point of intersection, and the lower limit was denoted  $\epsilon$ , with subscripts indicating the quantifier. This procedure returned the following values:  $\epsilon_{\omega} \sim .61$ ,  $\epsilon_{IR/IL} \sim .71$ ,  $\epsilon_{\eta} \sim .88$ , and  $\epsilon_{\Gamma} \sim .89$ . Note that an  $\epsilon$  of .5 means that both

Gaussians overlap completely, and an  $\epsilon$  of .84 means that the Gaussians overlap at the point where one of them attains its first standard deviation.

Based on this analysis, the most accurate quantifiers are the residual parameter and the line width of the 2D mode. It is surprising that  $\epsilon$  is so close to .5, for the central frequency and the asymmetry parameter. This could be the result of noise due to low integration times or the wide spectral resolution of  $8\text{cm}^{-1}$ .

It is important to mention that homogeneously stacked samples are quite rare. In fact, six out of six scanned samples contained both ABA and ABC domains. Additionally, we note that the sample analyzed in this paper is quite exquisite, in that the stacking domains are quite large and have nice, rectangular shapes. Other samples that we studied had many small domains with complex profiles. We must also note that not all stacking domains could be resolved. The laser spot in our Raman setup was 500nm in diameter, which is much larger than the length of a single hexagonal carbon ring. Furthermore, it is a possibility that small stacking domains are not displayed in our maps. This finding should be a concern (though hopefully not a deterrent) in future studies.

One important issue is the mechanism for formation of different stacking domains. It is rather unlikely that they arose in the process of cleaving graphite during mechanical exfoliation. Qualitatively, we must consider the strength of the van der Waal interactions that hold graphene layers together in graphite. While these forces are not strong enough to prevent easy peeling of layers, they are much stronger in the direction along the layer. Therefore, this would likely resist the layer-shifting processes that would presumably form these domains. Instead, it is more likely that three-dimensional domains were present in the bulk graphite before exfoliation, and that in cleaving graphene layers, we are simply exposing cross-sections of these domains.

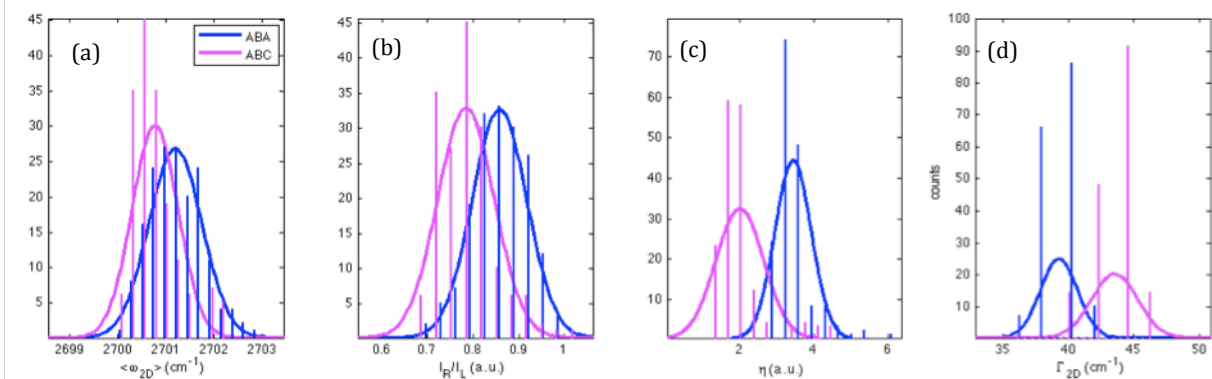


FIG. 4. Histograms and corresponding Gaussians for (a) the central frequency, (b) ratio of the integrated intensities of the right and left halves, (c) the residual parameter and (d) the line width of the 2D mode in ABA and ABC stacked domains. From these data, it is clear that the best way to map stacking domains is with the line width, whose histograms experience the least overlap. The amount of overlap in the other quantifiers is too significant to tell different stacking regions apart, with good confidence. See Table 1 in the Appendix for a summary of data presented here.



Now we must ask how homogeneous trilayers might be formed. It is possible that methods that involve the assembly of individual carbon atoms into sheets could produce homogeneous trilayers. These alternative synthetic routes are actually topics of intense research right now, with prominent methods involving chemical vapor deposition (CVD) [24] and epitaxial growth [25]. However, if such methods could produce homogeneous trilayers, it would be yet another task to discover a way to control stacking orders. Another possible way of creating homogeneous sheets might involve the heating of inhomogeneous samples. Molecular vibrations due to thermal excitation might force atoms to break out of their initial stacking order, and then into a homogeneous order upon cooling. Now that we have established methods that can be used to map stacking domains, it would be interesting to implement them on samples produced and treated in the ways described above.

## Conclusion

In this study it was found that the shape of the 2D mode in the Raman spectra of graphene trilayers is dependent upon the stacking geometry of graphene layers. ABC stacked samples show an asymmetric mode, while ABA stacked samples produce a more symmetric mode. By quantifying these shapes and using Raman imaging, it was possible for us to map stacking domains. A new parameter ( $\epsilon$ ) was introduced to measure the amount of overlap in our quantities of interest within ABA and ABC stacking domains. By using this parameter, it was found that the most accurate way to map stacking domains is with residual parameter (see Eq. (3)) and the line width. In a future study, it would be very interesting to perform Raman scanning with a spectral window around the D mode. It is likely that we could observe this mode in areas of stacking discontinuity, which could also prove useful in the mapping of stacking domains.

While we have found a way to map stacking domains, we have not formulated a theoretical explanation for why there is a difference in the 2D mode of ABA and ABC stacked trilayers. In addition, we have not fully understood the origin of more subtle features, such as the gradual red shifts that are present in the map representing the central frequency. Although these might be due to doping or strains, rigorous quantitative analysis has not been performed (see **Appendix A2** for further discussion).

Future work should extend our findings to higher order multilayers. Although it was not presented here, we found that the 2D mode in tetralayers and hexalayers also takes on different shapes in different stacking regions (see **Appendix A3**). While it may seem that studying higher order multilayers would become more complicated, this might not actually be the case. After considering mirror symmetries within the crystal, along with geometrically equivalent orders, the number of energetically favorable

stacking configurations declines tremendously. In fact, it is believed that there are only two energetically favorable tetralayers as well. Therefore, Raman might be effective for the characterization and mapping of stacking domains in higher order multilayers as well.

## Acknowledgements

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## Appendix

### A1. G Mode Analysis

In addition to studying the 2D mode, we briefly studied the G mode. Because the shape looked indistinguishable in ABA and ABC domains, we only computed the line width and the frequency of the mode. Although statistical analysis was not performed, we made several qualitative observations based on the colormaps presented in Fig. 5. From Fig. 5(a), it appears that the width of the G mode might be useful in determining different stacking orders. However, the frequency does not appear to be a useful parameter for this purpose, as ABC and ABA domains are essentially indistinguishable (see Fig. 5(b)).

### A2. Moderate features in the colormaps

In Fig. 3(b), we see the presence of a moderately varying feature. This is most easily seen in the angled, north-eastern region of the sample, within the ABA domain. In attempt to find an explanation for this feature, we briefly consider the effects of doping and strain on the Raman spectrum.

Studies in the literature show that doping causes the G mode to stiffen, while leaving the shape of the 2D mode unchanged. Therefore, the ratio of the integrated intensities of the two modes is a good indicator of the doping level. This calculation was performed with the result plotted in Fig. 6. Note that the horizontal lines are representative of instrumental malfunction. Irrespective of these artifacts, however, we do not see any features that resemble the one mentioned above.

Given that the 2D mode appears red-shifted in Fig. 3(c), it is natural for us to consider strain on the sample. Studies show that strain will cause the red shifting of both the 2D and G modes and will cause the G mode to split. While we do see a red shifting of the 2D mode in this region (Fig. 3(c)), the G mode does not appear to be

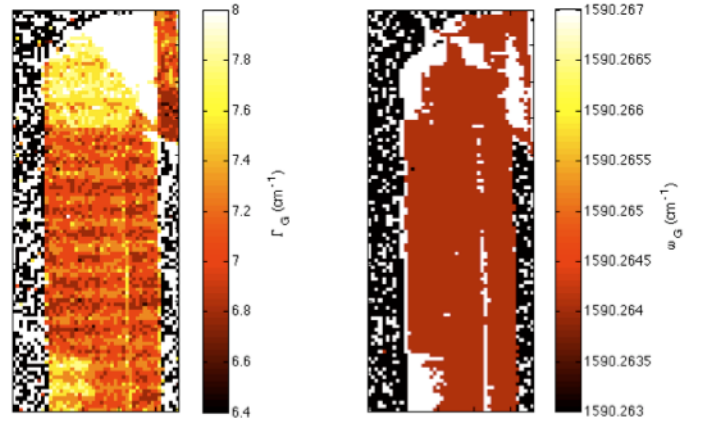


FIG. 5. (a) linewidth of the G mode and (b) frequency of the G mode, as determined by center of the Lorentzian function used to fit it. The horizontal lines in (a) are attributed to instrumental noise.

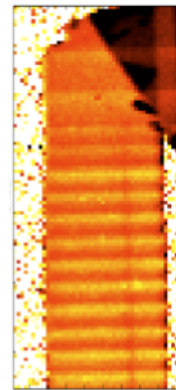


FIG. 6. Ratio of the integrated intensities of the 2D mode to the G mode. The horizontal lines may be attributed to instrumental noise. We do not see the gradually varying feature in Fig. 3(b), suggesting that doping might not be responsible for it. A color bar is not presented, as accurate numerical analysis here is not possible due to apparent laser intensity fluctuations.

shifted (see Fig. 5(b)). In addition, the line width of the G mode does not appear to be wider in that region (see Fig. 5(a)).

From this short, qualitative, analysis, it seems that neither strain nor doping are responsible for the gradually varying feature seen Fig. 3(b). However, without a rigorous quantitative study, we cannot make any conclusions. This would be an interesting topic for future studies.

### A3. Raman scattering on tetralayers and hexalayers

Raman scattering was also performed on various stacking domains in tetralayers and hexalayers (See Fig. 6). The resulting data implies that the 2D mode in higher order multilayer samples is also dependent upon the stacking geometry. And in fact, it appears that it is affected even more than in trilayer samples.

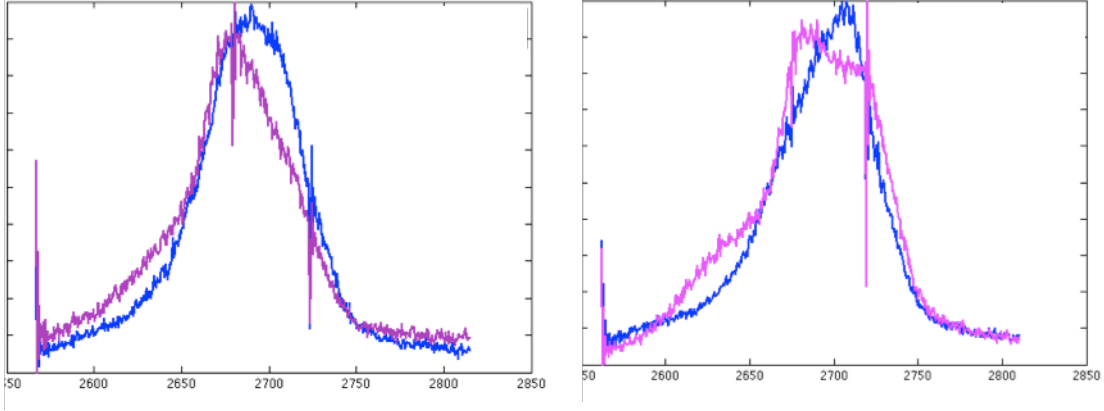


FIG. 6. 2D mode in differently stacked (a) tetralayers and in (b) hexalayers. The horizontal axis represents wavenumbers ( $\text{cm}^{-1}$ ) and the vertical axis the intensity (a.u.). Differences in stacking orders were determined by infrared spectroscopy. However, we do not claim a specific stacking order, as the number of possible configurations is quite large. There is a clear difference in the shapes of the modes indicating that Raman might prove to be a useful tool in the characterization of these materials.

### A4. Tables

TABLE 1. After spectral data was obtained, we determined the width at  $\frac{3}{4}$  max ( $\Gamma$ ), the residual parameter ( $\eta$ ), the central frequency ( $\langle\omega\rangle$ ), and the asymmetry parameter ( $I^L/I^R$ ). Histograms were then made for these quantities, and a Gaussian was used to fit them, assuming normal distributions. The mean ( $\mu$ ), the standard deviation ( $\sigma$ ), the point of intersection of the Gaussians ( $\chi$ ), and the integral from the point of intersection, to infinity, were calculated.

Q	$\Gamma_{ABA}$	$\Gamma_{ABC}$	$\eta_{ABA}$	$\eta_{ABC}$	$\langle\omega_{ABA}\rangle$	$\langle\omega_{ABC}\rangle$	$I^L/I^R_{ABA}$	$I^L/I^R_{ABC}$
$\mu$	$39.3\text{cm}^{-1}$	$43.6\text{cm}^{-1}$	3.46 (a.u.)	2.02 (a.u.)	$2701.2\text{cm}^{-1}$	$2700.8\text{cm}^{-1}$	.86(a.u.)	.79(a.u.)
$\sigma$	$1.4\text{cm}^{-1}$	$1.8\text{cm}^{-1}$	.49 (a.u.)	.64 (a.u.)	$.55\text{cm}^{-1}$	$.48\text{cm}^{-1}$	.06(a.u.)	.06(a.u.)
$\chi$	$41.3\text{cm}^{-1}$		2.78(a.u.)		$2701.1\text{cm}^{-1}$		.82(a.u.)	
$\frac{\int_{\chi}^{+\infty} G(Q)dQ}{\int_{-\infty}^{+\infty} G(Q)dQ}$	.93	.89	.92	.88	.61	.72	.74	.71

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## A5. MATLAB Code for data analysis

```
%% Raman Scanning Analysis Program by PAUL KLIMOV, Summer 2009.
close all; clear all; clc

%% THESE FEW LINES REQUIRE EDITING EVERY TIME A NEW FILE IS USED

load 2D_23X65_25mW_5s.txt;
load wavenumber.txt
Map=cell(46,110);
WN=wavenumber
WNsmooth=linspace(min(WN),max(WN),1000)
DATA=X2D_23X65_25mW_5s';
clear data1 data2 wavenumber
xdim=46 % the number of spectra in x direction
ydim=110 % the number of spectra in y direction

%while i load the data, i will find noise and subtract it out
NoiseInd=find(WN>1800&WN<2300); %this selects a region of noise
for i = 1:ydim;
    for k = 1:xdim;
        Map{k,i}=DATA(:,k+(i-1)*xdim);
        NoiseVals=Map{k,i}(NoiseInd);
        MeanNoise=mean(NoiseVals);
        Map{k,i}=Map{k,i}-MeanNoise;
        Map2{k,i}=spline(WN,Map{k,i},WNsmooth);

        %Normalize over 2D mode - this will be used later
        NormFactor=max(Map2{k,i}(find(WNsmooth>2500&WNsmooth<3000)));
        Normal2DMap{k,i}=Map2{k,i}/NormFactor;

        %Normalize over G mode - this will be used later
        NormFactorG=max(Map2{k,i}(find(WNsmooth>1000&WNsmooth<2100)));
        NormalGMap{k,i}=Map2{k,i}/NormFactorG;

    end
end
%% Fitting Lorentzian to the G mode Version 2

GInd=find(WNsmooth>1000&WNsmooth<2100);
PeakG=cell(xdim,ydim);
gamma=cell(xdim,ydim);
WidthG=cell(xdim,ydim);
CenterG=cell(xdim,ydim);
LorG=cell(xdim,ydim);
xG=WNsmooth(GInd)

for i = 1:ydim
    for k=1:xdim
        y=Map2{k,i}(GInd);

        [sigma,mu,AG]=mygaussfit(xG,y,.4); %optimized for .4
        Gauss=AG*exp( -(xG-mu).^2 / (2*sigma^2) ); % gaussian fit
        CenterG=xG(find(Gauss==max(Gauss))); % center of gaussian

        %Lorentzian fitting - finding gamma and the amplitude

        gammavec=linspace(0,50,200);
        peakvec=linspace(AG+5, AG-5,10);
        wavenumbervec=linspace(CenterG-3, CenterG+3,10);

        %residual=zeros(1,1000)
        % my fitting algorithm. It will scan through gammas, peak heights,
        % and frequencies to find the best fit. This part takes a long time
        % to run
        for u =1:10
            for l = 1:10
```



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```

        for j = 1:200
            testPeakG=peakvec(1);
            testgamma=gammavec(j);
            testwn=wavenumbervec(u);
            testLor=testPeakG*testgamma^2./((xG-testwn).^2+testgamma^2);
            residual(j,u,1)=sum(abs(y-testLor)); % residuals in a 3 dim matrix
        end
    end
end
%next line will find the minima of the 3 dimensional residual
%matrix and then from the indicies, my program will determine the
%corresponding gamma, frequency, and peak height.
[minj,minu,minl]=ind2sub(size(residual),find(residual==min(min(residual))));

gammaG{k,i}=gammavec(minj); %HWHM of Lorentzian
PeakG{k,i}=peakvec(minl); %Peak intensity of Lorentzian
wnG{k,i}=wavenumbervec(minu); %frequency of Lorentzian

% The following lines look for errors and get rid of them without
% crashing the program. They look for empty matrices, or matrices
% with more than one element, which can result from spectra with
% only noise.
if sum(size(gammaG{k,i}))>2
    gammaG{k,i}=0;
    PeakG{k,i}=0;
    wnG{k,i}=0;
    errormatG{k,i}=1;
end
if sum(size(gammaG{k,i}))==0
    gammaG{k,i}=0;
    PeakG{k,i}=0;
    wnG{k,i}=0;
    errormatG{k,i}=1;
end

FWHMGaussG(k,i)=2.3548*sigma; %The gaussian FWHM. This is not used anymore
LorG{k,i}=PeakG{k,i}*gammaG{k,i}^2./((xG-wnG{k,i}).^2+gammaG{k,i}^2); %the lorentzian fit
WidthG{k,i}=gammaG{k,i}; %HWHM of lorentzian
i
end
end
'done' %tells you when the program has finished running.
%It can take over 30 numbers depending on the resolution

%% run this to clear some unimportant variables and free up memory
clear residual testLor testwn testgamma testPeakG gammavec peakvec wavenumbervec
clear NoiseVals MeanNoise DATA Map
%% run this if you want to save out data to the current directory. You
%% Might want to add to these names to be more specific!
save WidthG2 WidthG
save LorG2 LorG
save PeakG2 PeakG
save gammaG2 gammaG
save wnG2 wnG

%% Run this if you want to load data from the current directory
%% If you changed names earlier, make sure to change these variables
load WidthG WidthG
load LorG LorG
load PeakG PeakG
load gammaG gammaG
load wnG wnG
%% Fitting Lorentzian to the 2D mode. Same code as for G mode.
TwoDInd=find(WNsmooth>2550&WNsmooth<2850);
%fit the 2D mode with a lorentzian
PeakTwoD=cell(xdim,ydim);
gamma=cell(xdim,ydim);
WidthTwoD=cell(xdim,ydim);
FWHMGaussTwoD=cell(xdim,ydim);
CenterTwoD=cell(xdim,ydim);
Lor2D=cell(xdim,ydim)
x2D=WNsmooth(TwoDInd)

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```

for i = 1:ydim
    for k=1:xdim
        y=Map2{k,i}(TwoDInd);

        [sigma,mu,A2D]=mygaussfit(x2D,y,.4); %optimized for .4
        Gauss=A2D*exp( -(x2D-mu).^2 / (2*sigma^2) );
        Center2D=x2D(find(Gauss==max(Gauss)));

        %Lorentzian fitting - finding gamma and the amplitude

        gammavec=linspace(0,50,200);
        peakvec=linspace(A2D+5, A2D-5,10);
        wavenumbervec=linspace(Center2D-3, Center2D+3,10);

        %residual=zeros(1,1000)
        for u =1:10
            for l = 1:10
                for j = 1:200
                    testPeak2D=peakvec(l);
                    testgamma=gammavec(j);
                    testwn=wavenumbervec(u);
                    testLor=testPeak2D*testgamma^2./((x2D-testwn).^2+testgamma^2);
                    residual(j,u,l)=sum(abs(y-testLor));
                end
            end
        end
        [minj,minu,minl]=ind2sub(size(residual),find(residual==min(min(min(residual)))));

        gamma2D{k,i}=gammavec(minj);
        Peak2D{k,i}=peakvec(minl);
        wn2D{k,i}=wavenumbervec(minu);

        if sum(size(gamma2D{k,i}))>2
            gamma2D{k,i}=0;
            Peak2D{k,i}=0;
            wn2D{k,i}=0;
            errormat2D{k,i}=1;
        end
        if sum(size(gamma2D{k,i}))==0
            gamma2D{k,i}=0;
            Peak2D{k,i}=0;
            wn2D{k,i}=0;
            errormat2D{k,i}=1;
        end
        FWHMGaussG(k,i)=2.3548*sigma;
        Lor2D{k,i}=Peak2D{k,i}*gamma2D{k,i}^2./((x2D-wn2D{k,i}).^2+gamma2D{k,i}^2);
        Width2D{k,i}=gamma2D{k,i};
    end
end
end
'done'
%% Run this to save out 2D mode information
save Width2D_2 Width2D
save Lor2D_2 Lor2D
save Peak2D_2 Peak2D
save gamma2D_2 gamma2D
save wn2D_2 wn2D
%% Run this to load 2D mode information
load Width2D_2 Width2D
load Lor2D_2 Lor2D
load Peak2D_2 Peak2D
load gamma2D_2 gamma2D
load wn2D_2 wn2D
%% Run this to clear out some memory
clear A2D DATA Gauss MeanNoise NoiseInd NoiseVals NormFactor NormFactorG
clear testLor sigma residual peakvec testPeak2D testgamma testwn wavenumbervec
%% Integrated intensity Gmode.
Gintegrationind=find(WNsmooth>1570&WNsmooth<1610); %finds region of integration
TwoDintegrationind=find(WNsmooth>2620&WNsmooth<2780); %finds region of integration

for i = 1:ydim

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    for k=1:xdim
        IntegratedG(k,i)=sum(abs(Map2{k,i}(Gintegrationind))));
        Integrated2D(k,i)=sum(abs(Map2{k,i}(TwoDintegrationind))));
        Integrated2DNorm(k,i)=sum(Normal2DMap{k,i}(TwoDintegrationind));
    end
end
Ratio2DtoG=Integrated2D./IntegratedG; % The integrated intensities ratio
%% Save Integrated Intensity data
save IntegratedG IntegratedG
save Integrated2D Integrated2D
save Ratio2DtoG Ratio2DtoG
%% Moments calculations
WN2DcmInd=find(WNsmooth>2670&WNsmooth<2737)

for i = 1:ydim
    for k = 1:xdim
        Intensitysum(k,i)=sum(Normal2DMap{k,i}(WN2DcmInd));

        %first moment
        WNCm(k,i)=sum(WNsmooth(WN2DcmInd).*Normal2DMap{k,i}(WN2DcmInd))/Intensitysum(k,i);

    end
end

climWNCm=[2700 2705]
imagesc(WNCm,climWNCm)
colorbar; axis equal tight
title('first moment 2D')
set(gcf,'color',[1,1,1]); colormap hot

%the following plot gives random plots so you can see the region of
%integration
% figure
% for p = 1:9
%     subplot(3,3,p)
%     plot(WNsmooth(WN2DcmInd),...
%         Normal2DMap{floor(100*rand(1)+1),floor(40*rand(1)+1)}(WN2DcmInd))
%     axis([2670,2737,0,1])
% end
%% Save Moments
save WNCm WNCm
%% Plots
%%
%%
%%
%% Gmode Plots
subplot(1,2,1)
climwidth=[6.4 8];
imagesc(cell2mat(WidthG)',climwidth)
colormap hot
colorbar
ylabel(texlabel('Gamma_G (cm^-1)'))
set(gcf,'color',[1,1,1]); axis equal tight
set(gca,'YTickLabel',[]);
set(gca,'XTickLabel',[]);

%these next loops get rid of 'broken' data points, so we can plot the G
%frequencies
for i = 1:ydim
    for k = 1:xdim
        if length(find(LorG{k,i}==max(LorG{k,i})))>1
            shiftG(k,i)=0
            continue
        end
        shiftG(k,i)=wnG{find(LorG{k,i}==max(LorG{k,i}))};
    end
end

subplot(1,2,2)
climshiftG= [1590.2641 1590.2641]
imagesc(shiftG',climshiftG)
colorbar;set(gcf,'color',[1,1,1])

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```

colormap hot; axis equal tight
ylabel(texlabel('omega_G (cm^-1)'))
set(gca, 'YTickLabel', []);
set(gca, 'XTickLabel', []);

figure
climintensity=[1475 1760];
imagesc(cell2mat(PeakG),climintensity)
colorbar
title('G Mode Intensity')
set(gcf, 'color', [1,1,1])
colormap hot

%2D to G integrated intensity
figure
subplot(3,1,1)
climratio=[1,1.76]*10^4
imagesc(IntegratedG,climratio)
colorbar;title('IG');colormap hot;set(gcf, 'color', [1,1,1])

subplot(3,1,2)
climratio=[2,5]*10^4
imagesc(Integrated2D,climratio)
colorbar;title('I2D');colormap hot;set(gcf, 'color', [1,1,1])

subplot(3,1,3)
climratio=[2,4]
imagesc(Integrated2D./IntegratedG,climratio)
colorbar;title('I2D/IG');colormap hot;set(gcf, 'color', [1,1,1])
%% 2D mode plots

figure
climswidthD = [ 24 29 ]
imagesc(cell2mat(Width2D),climswidthD)
title('2D Mode Lorentzian Peak Width')
colorbar; colormap hot; axis equal tight
set(gcf, 'color', [1,1,1])

figure
climscenderD=[2690 2705]
imagesc(cell2mat(wn2D),climscenderD)
title('2D Mode Peak Center')
colorbar; colormap hot; axis equal tight
set(gcf, 'color', [1,1,1])

%% Widths at different heights for 2D mode and one G. This measures the
%% spectra directly, not the Lorentzians corresponding to the data
TwoDInd=find(WNsmooth>2550&WNsmooth<2850);
GInd2=find(WNsmooth>1570&WNsmooth<1620);
for i = 1:ydlim
    for k = 1:xdim
        fiftyInd=find(Normal2DMap{k,i}(TwoDInd)>.5);
        seventyfiveInd=find(Normal2DMap{k,i}(TwoDInd)>.75);
        eightyInd=find(Normal2DMap{k,i}(TwoDInd)>.80);
        seventyfiveIndG=find(NormalGMap{k,i}(GInd2)>.5);

        if isempty(seventyfiveInd)==1
            errorind(k,i)=1
            continue
        end
        if isempty(fiftyInd)==1
            errorind(k,i)=1
            continue
        end
        if isempty(eightyInd)==1
            errorind(k,i)=1
            continue
        end
        if isempty(seventyfiveIndG)==1
            errorindG(k,i)=1
            continue
        end
    end
end

```

---

```

        fiftywidth(k,i)=abs(WNsmooth(min(fiftyInd))-WNsmooth(max(fiftyInd)));
        seventyfivewidth(k,i)=abs(WNsmooth(min(seventyfiveInd))-WNsmooth(max(seventyfiveInd)));
        % eightywidth(k,i)=abs(WNsmooth(min(eightyInd))-WNsmooth(max(eightyInd)));
        seventyfivewidthG(k,i)=abs(WNsmooth(min(seventyfiveIndG))-WNsmooth(max(seventyfiveIndG)));
    end
end
fiftywidth(find(errorind==1))=100
seventyfivewidth(find(errorind==1))=100
eightywidth(find(errorind==1))=100

figure
climsfifty=[50 77]
imagesc(fiftywidth,climsfifty)
title('fifty width')
colorbar
axis equal tight
set(gcf,'color',[1,1,1])
colormap hot
% subplot(3,2,2)
% plot(6:1:35, fiftywidth(7,6:end))
% axis tight

figure
climsseventyfive=[34 49]
imagesc(seventyfivewidth,climsseventyfive)
title('seventy five width')
colorbar
axis equal tight; colormap hot
set(gcf,'color',[1,1,1])

figure
hist(seventyfivewidth);axis([0 100 0 80])

% %
% % subplot(3,2,4)
% % plot(6:1:35, seventyfivewidth(7,6:end))
% % axis tight
%
% figure
% climsseighty=[10 40]
% imagesc(eightywidth,climsseighty)
% title('eighty width')
% colorbar
% axis equal tight
% set(gcf,'color',[1,1,1])
% colormap winter
% % subplot(3,2,6)
% % plot(6:1:35, eightywidth(7,6:end))
% % axis tight

%
% figure
%
climsseventyfiveG=[8 19]
imagesc(seventyfivewidthG,climsseventyfiveG)
title('fifty width G')
colorbar
axis equal tight
set(gcf,'color',[1,1,1])
colormap hot
%% Final Plots

subplot(2,3,1)
WNcm(30:34,32)=0% these types of changes are here to draw a square where data was taken
WNcm(30:34,36)=0% in the later part of the program
WNcm(34,32:36)=0
WNcm(30,32:36)=0

WNcm(34:38,43)=0
WNcm(34:38,47)=0
WNcm(34,43:47)=0

```



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```

WNcm(38,43:47)=0

imagesc(WNcm,[2700,2706])
colorbar
set(gcf,'color',[1,1,1]); colormap hot
ylabel(texlabel('Omega_2_D (cm^-1)'))
set(gca,'YTickLabel',[])
set(gca,'XTickLabel',[])

subplot(2,3,2)
WidthGPlot=cell2mat(WidthG)
WidthGPlot(30:34,32)=0
WidthGPlot(30:34,36)=0
WidthGPlot(34,32:36)=0
WidthGPlot(30,32:36)=0

WidthGPlot(34:38,43)=0
WidthGPlot(34:38,47)=0
WidthGPlot(34,43:47)=0
WidthGPlot(38,43:47)=0

climwidth=[6.8 8.5];
imagesc(WidthGPlot,climwidth)
colormap hot
colorbar
set(gcf,'color',[1,1,1])
ylabel(texlabel('Gamma_G (cm^-1)'))
set(gca,'YTickLabel',[])
set(gca,'XTickLabel',[])

wnGPlot=cell2mat(wnG)
wnGPlot(30:34,32)=0
wnGPlot(30:34,36)=0
wnGPlot(34,32:36)=0
wnGPlot(30,32:36)=0

wnGPlot(34:38,43)=0
wnGPlot(34:38,47)=0
wnGPlot(34,43:47)=0
wnGPlot(38,43:47)=0
subplot(2,3,3)
climcenter=[1587 1593];
imagesc(wnGPlot,climcenter)
colorbar
set(gcf,'color',[1,1,1])
colormap hot
ylabel(texlabel('omega_G (cm^-1)'))
set(gca,'YTickLabel',[])
set(gca,'XTickLabel',[])

subplot(2,3,4)
Width2DPlot=cell2mat(Width2D)
Width2DPlot(30:34,32)=0
Width2DPlot(30:34,36)=0
Width2DPlot(34,32:36)=0
Width2DPlot(30,32:36)=0

Width2DPlot(34:38,43)=0
Width2DPlot(34:38,47)=0
Width2DPlot(34,43:47)=0
Width2DPlot(38,43:47)=0
climswidthD = [ 24 30 ]
imagesc(Width2DPlot,climswidthD)
colorbar; colormap hot
set(gcf,'color',[1,1,1])
ylabel(texlabel('Gamma_2_D (cm^-1)'))
set(gca,'YTickLabel',[])
set(gca,'XTickLabel',[])

subplot(2,3,5)

```

---

```

wn2DPlot=cell2mat(wn2D)
wn2DPlot(30:34,32)=0
wn2DPlot(30:34,36)=0
wn2DPlot(34,32:36)=0
wn2DPlot(30,32:36)=0

wn2DPlot(34:38,43)=0
wn2DPlot(34:38,47)=0
wn2DPlot(34,43:47)=0
wn2DPlot(38,43:47)=0
climscenterD=[2693 2710]
imagesc(wn2DPlot,climscenterD)
colorbar; colormap hot
set(gcf,'color',[1,1,1])
ylabel(texlabel('omega_2_D (cm^-1)'))
set(gca,'YTickLabel',[])
set(gca,'XTickLabel',[])

subplot(2,3,6)
climratio=[2,3.1]
imagesc(Integrated2D./IntegratedG,climratio)
colorbar;ylabel('I_2_D/I_G (a.u.)');colormap hot;set(gcf,'color',[1,1,1])
set(gca,'YTickLabel',[])
set(gca,'XTickLabel',[])

%% Calculation of variations of intensity. to determine magnitude of
%% effect. The grid is shown in the figures above.

DeltaMoment=mean(mean([WNcm(15:20,20:25)- WNcm(20:25,50:55)]))
PercentMoment=mean(mean(DeltaMoment./WNcm(30:34,32:36)*100))
DeltaWidthG=mean(mean([cell2mat(WidthG(30:34,32:36))-cell2mat(WidthG(34:38,43:47))]))
PercentWidthG=mean(mean([cell2mat(WidthG(30:34,32:36))-
cell2mat(WidthG(34:38,43:47))]./cell2mat(WidthG(30:34,32:36))*100))
DeltafreqG=mean(mean([cell2mat(wnG(29:33,32:36))-cell2mat(wnG(34:38,43:47))]))
PercentfreqG=mean(mean([cell2mat(wnG(29:33,32:36))-
cell2mat(wnG(34:38,43:47))]/cell2mat(wnG(29:33,32:36))*100))
DeltaWidth2D=mean(mean([cell2mat(Width2D(30:34,32:36))-cell2mat(Width2D(34:38,43:47))]))
PercentWidth2D=mean(mean([cell2mat(Width2D(30:34,32:36))-
cell2mat(Width2D(34:38,43:47))]./cell2mat(Width2D(30:34,32:36))*100))
Deltafreq2D=mean(mean([cell2mat(wn2D(30:34,32:36))-cell2mat(wn2D(34:38,43:47))]))
Percentfreq2D=mean(mean([cell2mat(wn2D(30:34,32:36))-
cell2mat(wn2D(34:38,43:47))]./cell2mat(wn2D(30:34,32:36))*100))

%% The 2D and G mode averaged in the same regions as shown in the figures
%% above.
%Normal2DMap
% ABAG=zeros(1,1000)
ABA2D=zeros(1,1000)
%
% ABCG=zeros(1,1000)
ABC2D=zeros(1,1000)

%LorABAG=zeros(1,408)
%LorABCG=zeros(1,408)

%LorABA2D=zeros(1,141)
%LorABC2D=zeros(1,141)

for i = 1:5
    for j = 1:10
        % ABA stuff
        tempspec=NormalGMap{30+(i-1),32+j-1}; %these are the ABA indicies
        % ABAG = ABAG + tempspec;
        tempspec=Normal2DMap{11+(i-1),18+j-1};
        ABA2D= ABA2D + tempspec;

        % tempspec=LorG{30+(i-1),32+j-1};
        % LorABAG=LorABAG+tempspec
        % tempspec=Lor2D{30+(i-1),32+j-1};
        % LorABA2D=LorABA2D+tempspec

```

---

```

%
% ABC stuff
% tempspec=NormalGMap{34+(i-1),43+j-1};
% ABCG = ABCG + tempspec;
% tempspec=Normal2DMap{15+(i-1),60+j-1};
% ABC2D= ABC2D + tempspec;

% tempspec=LorG{34+(i-1),43+j-1};
% LorABCG=LorABCG+tempspec
% tempspec=Lor2D{34+(i-1),43+j-1};
% LorABC2D=LorABC2D+tempspec

end
end

% ABAG=ABAG/max(ABAG);
% ABCG=ABCG/max(ABCG);
% ABA2D=ABA2D/max(ABA2D);
% ABC2D=ABC2D/max(ABC2D);
% LorABCG=LorABCG/max(LorABCG);
% LorABAG=LorABAG/max(LorABAG);
% LorABC2D=LorABC2D/max(LorABC2D);
% LorABA2D=LorABA2D/max(LorABA2D);

% subplot(1,4,1)
% plot(WNsmooth,ABAG,WNsmooth,ABCG,'m','linewidth',2);axis([1560,1620,0,1]);legend('ABA','ABC')
% set(gca,'YTickLabel',[]);xlabel('cm^-1')
% subplot(1,4,2);
% plot(xG,LorABAG,xG,LorABCG,'m','linewidth',2);axis([1560,1620,0,1]);
% set(gca,'YTickLabel',[]);xlabel('cm^-1')
% subplot(1,4,3);
% plot(WNsmooth,ABA2D,WNsmooth,ABC2D,'m','linewidth',2);axis([2600,2800,0,1]);
% set(gca,'YTickLabel',[]);xlabel('cm^-1'); legend('ABA','ABC')

% plot(x2D,LorABA2D,x2D,LorABC2D,'m','linewidth',2);axis([2600,2800,0,1]);
% set(gcf,'color',[1,1,1]);set(gca,'YTickLabel',[]);xlabel('cm^-1')
% % Now, load the Lorentzians

%% Statistical analysis for width
AWidth=reshape(seventyfiveWidth(10:22,15:27),[prod(size(seventyfiveWidth(10:22,15:27))) 1])
BWidth=reshape(seventyfiveWidth(10:22,53:65),[prod(size(seventyfiveWidth(10:22,15:27))) 1])
XWidth=linspace(20,60,140)

[HAWidth,XAWidth]=hist(AWidth,11)
[HBWidth,XBWidth]=hist(BWidth,19)

XAWidth(1)-XAWidth(2)
XBWidth(1)-XBWidth(2)

YAWidth=88*sqrt(1/2/pi/std(AWidth)^2)*exp(-((XWidth-mean(AWidth)).^2)/(2*std(AWidth)^2))
histfit(AWidth,11); hold on
plot(XWidth,YAWidth,XAWidth,HAWidth,'o');
hold off

YBWidth=88*sqrt(1/2/pi/std(BWidth)^2)*exp(-((XWidth-mean(BWidth)).^2)/(2*std(BWidth)^2))
histfit(BWidth,19); hold on
plot(XWidth,YBWidth,XBWidth,HBWidth,'o');
hold off

NormAWidth=YAWidth/sum(YAWidth)
NormBWidth=YBWidth/sum(YBWidth)

```

---

```

plot(XWidth,YAWidth,XWidth,YBWidth)
plot(XWidth,NormAWidth,XWidth,NormBWidth)

ABA.widthmean=mean(AWidth)
ABA.widthstd=std(AWidth)
ABA.widthintersect=41.3376
ABA.widthintegral=sum(NormAWidth(find(XWidth>ABA.widthintersect)))

ABC.widthmean=mean(BWidth)
ABC.widthstd=std(BWidth)
ABC.widthintegral=sum(NormBWidth(find(XWidth<ABA.widthintersect)))

%% histograms in the grid for first moment
AMom=reshape(WNcm(10:22,15:27),[prod(size(WNcm(10:22,15:27))) 1])
BMom=reshape(WNcm(10:22,53:65),[prod(size(WNcm(10:22,15:27))) 1])
XMom=linspace(2690,2710,400)

[HAMom,XAMom]=hist(AMom,13);
[HBMom,XBMom]=hist(BMom,10);

XAMom(1)-XAMom(2)
XBMom(1)-XBMom(2)

YAMom=37*sqrt(1/2/pi/std(AMom)^2)*exp(-((XMom-mean(AMom)).^2)/(2*std(AMom)^2))
histfit(AMom,13); hold on
plot(XMom,YAMom,XAMom,HAMom,'o');
hold off

YBMom=36*sqrt(1/2/pi/std(BMom)^2)*exp(-((XMom-mean(BMom)).^2)/(2*std(BMom)^2))
histfit(BMom,10); hold on
plot(XMom,YBMom,XBMom,HBMom,'o');
hold off

NormAMom=YAMom/sum(YAMom)
NormBMom=YBMom/sum(YBMom)

plot(XMom,YAMom,XMom,YBMom)
plot(XMom,NormAMom,XMom,NormBMom)

ABA.mommean=mean(AMom)
ABA.momstd=std(AMom)
ABA.momintersect=2701.0637 % this has to be entered manually
ABA.momintegral=sum(NormAMom(find(XMom>ABA.momintersect)))

ABC.mommean=mean(BMom)
ABC.momstd=std(BMom)
ABC.momintegral=sum(NormBMom(find(XMom<ABA.momintersect)))

%%
AFreq=reshape(cell2mat(wn2D(10:22,15:27)),[prod(size(cell2mat(wn2D(10:22,15:27)))) 1])
BFreq=reshape(cell2mat(wn2D(10:22,53:65)),[prod(size(cell2mat(wn2D(10:22,15:27)))) 1])
XFreq=linspace(2690,2710,400)

[HAFreq,XAFreq]=hist(AFreq,15);
[HBFreq,XBFreq]=hist(BFreq,11);

XAFreq(1)-XAFreq(2)
XBFreq(1)-XBFreq(2)

YAFreq=89*sqrt(1/2/pi/std(AFreq)^2)*exp(-((XFreq-mean(AFreq)).^2)/(2*std(AFreq)^2))
histfit(AFreq,15); hold on
plot(XFreq,YAFreq,XAFreq,HAFreq,'o');
hold off

```

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YBFreq=89*sqrt(1/2/pi/std(BFreq)^2)*exp(-(XFreq-mean(BFreq)).^2)/(2*std(BFreq)^2))
histfit(BFreq,11); hold on
plot(XFreq,YBFreq,XBFreq,HBFreq,'o');
hold off

NormAFreq=YAFreq/sum(YAFreq)
NormBFreq=YBFreq/sum(YBFreq)

plot(XFreq,YAFreq,XFreq,YBFreq)
plot(XFreq,NormAFreq,XFreq,NormBFreq)

ABA.freqmean=mean(AFreq)
ABA.freqstd=std(AFreq)
ABA.freqintersect=2696.1463 % this has to be entered manually
ABA.freqintegral=sum(NormAFreq(find(XFreq>ABA.freqintersect)))

ABC.freqmean=mean(BFreq)
ABC.freqstd=std(BFreq)
ABC.freqintegral=sum(NormBFreq(find(XFreq<ABA.freqintersect)))

%% Final Histogram plots
subplot(1,4,4)
plot(XWidth,YAWidth,'b',XWidth,YBWidth,'m',XAWidth,HAWidth,'bo',...
     XBWidth,HBWidth,'mo','linewidth',3)

ylabel('counts')
xlabel(texlabel('Gamma_2_D (cm^-1)'))
subplot(1,4,1)
plot(XMom,YAMom,'b',XMom,YBMom,'m',XAMom,HAMom,'bo',...
     XBMom,HBMom,'mo','linewidth',3)
legend('ABA','ABC')
xlabel(texlabel('<omega_2_D> (cm^-1)'))
subplot(1,4,2)
plot(XRat,YARat,'b',XRat,YBRat,'m',XARat,HARat,'bo',...
     XBRat,HBRat,'mo','linewidth',3)
xlabel(texlabel('I_R/I_L (a.u.)'))
set(gcf,'color',[1,1,1])
subplot(1,4,3)
plot(XSum,YASum,'b',XSum,YBSum,'m',XASum,HASum,'bo',...
     XBSum,HBSum,'mo','linewidth',3)
xlabel(texlabel('eta (a.u.)'))
set(gcf,'color',[1,1,1])

%% Multiple gaussian fits
for i = 1:ydlim;
    for k = 1:xdim;
        Data=Normal2DMap{k,i};
        Data=Data(TwoDInd);
        [u,sig,t,iter]=fit_mix_gaussian(Data',2);
        U{k,i}=u;
        SIG{k,i}=sig;
        DIST(k,i)=abs(u(1)-u(2));
    end
end
end
%%

imagesc(DIST',[.4,.52]);axis equal tight; colorbar

%% Integrating two halves

for i = 1:ydlim;
    for k=1:xdim

        Data=Normal2DMap{k,i}(TwoDInd);
        newindices=find(Data>.15);

        newdata=Data(newindices);

```



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```

centerindex=round(length(newindices)/2);
LeftInt=sum(newdata(1:centerindex-3));
if sum(size(newdata))==1
    continue
end
RightInt=sum(newdata(centerindex+3:end));
Ratio(k,i)=LeftInt/RightInt;
end
end

imagesc(Ratio',[.5,1]); colorbar; axis equal tight; colormap hot

%% histograms in the grid for Ratio
ARat=reshape(Ratio(10:22,15:27),[prod(size(Ratio(10:22,15:27))) 1]);
BRat=reshape(Ratio(10:22,53:65),[prod(size(Ratio(10:22,15:27))) 1]);
XRat=linspace(0,2,400);

[HARat,XARat]=hist(ARat,10);
[HBRat,XBRat]=hist(BRat,11);

XARat(1)-XARat(2)
XBRat(1)-XBRat(2)

YARat=4.9*sqrt(1/2/pi/std(ARat)^2)*exp(-((XRat-mean(ARat)).^2)/(2*std(ARat)^2))
histfit(ARat,10); hold on
plot(XRat,YARat,XARat,HARat,'o');
hold off

YBRat=5.1*sqrt(1/2/pi/std(BRat)^2)*exp(-((XRat-mean(BRat)).^2)/(2*std(BRat)^2))
histfit(BRat,11); hold on
plot(XRat,YBRat,XBRat,HBRat,'o');
hold off

NormARat=YARat/sum(YARat)
NormBRat=YBRat/sum(YBRat)

plot(XRat,YARat,XRat,YBRat)
plot(XRat,NormARat,XRat,NormBRat)

ABA.ratmean=mean(ARat)
ABA.ratstd=std(ARat)
ABA.ratintersect=2.78 % this has to be entered manually
ABA.ratintegral=sum(NormARat(find(XRat>ABA.ratintersect)))

ABC.ratmean=mean(BRat)
ABC.ratstd=std(BRat)
ABC.ratintegral=sum(NormBRat(find(XRat<ABA.ratintersect)))

%% histograms in the grid for SUM
ASum=reshape(SUMDAT(10:22,15:27),[prod(size(SUMDAT(10:22,15:27))) 1]);
BSum=reshape(SUMDAT(10:22,53:65),[prod(size(SUMDAT(10:22,15:27))) 1]);
XSum=linspace(0,5,400);

[HASum,XASum]=hist(ASum,10);
[HBSum,XBSum]=hist(BSum,10);

XASum(1)-XASum(2)
XBSum(1)-XBSum(2)

YASum=54*sqrt(1/2/pi/std(ASum)^2)*exp(-((XSum-mean(ASum)).^2)/(2*std(ASum)^2))
histfit(ASum,10); hold on
plot(XSum,YASum,XASum,HASum,'o');
hold off

YBSum=52*sqrt(1/2/pi/std(BSum)^2)*exp(-((XSum-mean(BSum)).^2)/(2*std(BSum)^2))

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```

histfit(BSum,10); hold on
plot(XSum,YBSum,XBSum,HBSum,'o');
hold off

NormASum=YASum/sum(YASum)
NormBSum=YBSum/sum(YBSum)

plot(XSum,YASum,XSum,YBSum)
plot(XSum,NormASum,XSum,NormBSum)

ABA.summean=mean(ASum)
ABA.sumstd=std(ASum)
ABA.sumintersect=2.78 % this has to be entered manually
ABA.sumintegral=sum(NormASum(find(XSum>ABA.sumintersect)))

ABC.summean=mean(BSum)
ABC.sumstd=std(BSum)
ABC.sumintegral=sum(NormBSum(find(XSum<ABA.sumintersect)))

%% Divide everything by the smooth 2D Mode
smooth2Dmode=Normal2DMap{15,51}(TwoDInd)

for i = 1:ydlim;
    for k=1:xlim
        Data=Normal2DMap{k,i}(TwoDInd);
        Ratio(k,i)=sum(abs(Data-smooth2Dmode));
    end
end

imagesc(SUMDAT,[0,8]);colorbar; colormap hot

%%
plot(WNsmooth(TwoDInd),Normal2DMap{15,51}(TwoDInd))

%% Plots for long strip 2

subplot(1,4,4)
climsseventyfive=[34 49]
imagesc(seventyfivewidth',climsseventyfive)
colorbar; colormap hot; axis equal tight
set(gcf,'color',[1,1,1]);set(gca,'YTickLabel',[]);
set(gca,'XTickLabel',[]);
ylabel(texlabel('Gamma_2D (cm^-^1)'))
%set(gca,'YTickLabel',[]);xlabel('cm^-^1')

subplot(1,4,3)
imagesc(SUMDAT',[0,8]); axis equal tight
colorbar; colormap hot;
set(gcf,'color',[1,1,1]);set(gca,'YTickLabel',[]);
set(gca,'XTickLabel',[]);
ylabel(texlabel('eta (a.u.)'))

subplot(1,4,1)
climWNcm=[2700 2705]
imagesc(WNcm',climWNcm)
colorbar; axis equal tight
ylabel(texlabel('<omega_2D> (cm^-^1)'))
set(gcf,'color',[1,1,1]); colormap hot;set(gca,'YTickLabel',[]);
set(gca,'XTickLabel',[]);

subplot(1,4,2)
imagesc(Ratio',[.5,1]); colorbar; axis equal tight; colormap hot
ylabel(texlabel('I_R/I_L (a.u.)'))
set(gcf,'color',[1,1,1]); colormap hot;set(gca,'YTickLabel',[]);
set(gca,'XTickLabel',[]);

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